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Editorial Forward

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With the availability of next generation sequencing technology, there is a tremendous need for development of novel tools, algorithms and methodologies for extracting useful information and knowledge from exponentially growing data. This need has catalyzed active research in the overlapping fields of Machine Learning (ML) and Artificial Intelligence (AI). Conventional linear and nonlinear tools for classification, regression and data driven modeling are being replaced on a rapid scale by newer techniques. While the linear techniques are not applicable for inherently nonlinear problems, newer methods serve as attractive alternatives for solving large scale and real life problems as in chemo and bioinformatics. Neural networks, based on the interconnected network of neurons, are one such tool which has been in the forefront of desirable list of tools in computational biology research. Support Vector Machine (SVM) classifiers are a set of universal feed-forward network based classification algorithms that have been formulated rigorously from statistical learning theory and structural risk minimization principle. The SVM-based regression closely follows the classification methodology while it has now been routinely used for prediction of gene and protein functions, microarray analysis in identification of different diseases including several cancer types etc. With the availability of structures the focus is now on structure based identification of drug targets and there are several methodologies which provide a large number of geometrical features, energy based and knowledge based features. For prediction algorithms to work efficiently, we thus need to extract and provide the most informative features to them. Intelligent algorithms and heuristic methodologies in conjunction with powerful classifiers like SVM can effectively extract informative features and identify functions like ligand binding sites and potential drug targets.

In the first issue of the journal International journal of computational Biology (IJCB) there are 6 research articles which employ different protocols involved in AI and ML methods using important applications in chemo and bioinformatics.

Vivekanand et al. [1] have suggested a protocol for **Accurate Demarcation of Protein Domain Linkers which is based on Structural Analysis of Linker Probable Region**. By applying and validating this method on 725 continuous multi-domain proteins, the authors have showed the usability of this approach in combination with supervised/sequence based linker prediction.

In the second paper, Chen et al. [2] discuss solving sequence-structure paradox. The authors showed how effectively **Protein Local Tertiary Structure can be predicted by Super Granule Support Vector Machines utilizing Chou-Fasman Parameters**.

The paper titled "**TpPred: A tool for hierarchical prediction of transport proteins using cluster of neural networks and sequence derived features**" by Jain et al.[3] is a very interesting tool, developed on a three level hierarchical classification using cascade of neural networks from sequence derived features. It gives overall success rates for all the three layers which turns out to be higher than 65%, on very stringent benchmark datasets.

Next, Pugalenthi et al. [4] have reported on the development of a tool detailed in "**iFace: a bioinformatics tool for the analysis of protein-protein interface**" which analyzes the protein-protein interfaces using three-dimensional structural information. The tool iFace identifies PPI sites and various interactions that contribute to the specificity and strength of the protein complex.

The first cheminformatics paper of this issue is a work by Vyas et al.[5] where they have detailed a comparative study between **several parametric and non-parametric ML approaches like ANN, k-nearest neighbour (kNN), decision trees, partial least squares**, etc. Furthermore, a case study involving the use of SVM method for screening molecules for cancer therapy has been discussed and reported.

Another article on a cheminformatics application has been reported by Sengupta et al. [6] which uses **SVM for Virtual Screening of ligand molecules**. They have shown how effectively the statistical learning theory can be used for several applications in virtual screening.

That said, I am very much pleased to release the first issue of IJCB with some very good research articles as discussed aforementioned. With a detailed view of the cutting edge machine learning algorithms, we believe this issue sheds light on a wide area of applications in the area of SVM. We hope the articles would have caught the interest of the readers whilst welcoming you to contribute articles in this journal.

Wishing you all a very good readership, I remain

REFERENCE

[1] Vivekanand et al. Accurate Demarcation of Protein Domain Linkers Based on Structural Analysis of Linker Probable Region. IJCB. 2012; Volume 1 (Issue 1): Page 03-13.
[2] Chen et al. Protein Local Tertiary Structure Prediction by Super Granule Support Vector Machines with Chou-Fasman Parameter. IJCB. 2012; Volume 1 (Issue 1): Page 14-27.
[3] Jain et al. TpPred: A Tool for Hierarchical Prediction of Transport Proteins Using Cluster of Neural Networks and Sequence Derived Features. IJCB. 2012; Volume 1 (Issue 1): Page 28-36.
[4] Pugalenthi et al. iFace: A Bioinformatics Tool for the Analysis of Protein-Protein Interface. IJCB. 2012; Volume 1 (Issue 1): Page 37-42.
[5] Vyas et al. Applications of Support Vector Machines as a Robust tool in High Throughput Virtual Screening. IJCB. 2012; Volume 1 (Issue 1): Page 43-55.
[6] Sengupta et al. Application of Support Vector Machines in Virtual Screening. IJCB. 2012; Volume 1 (Issue 1): Page 56-62.